Symmetry unrestricted Skyrme mean-field study of heavy nuclei

Wouter Ryssens, M. Bender & P.-H. Heenen

ULB

23rd of November

Summary

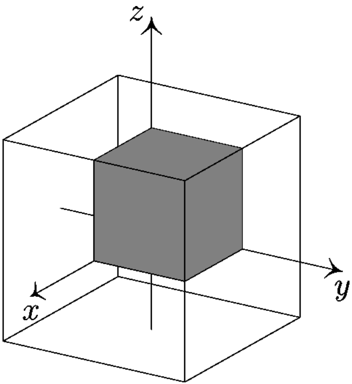
Ingredients

- Skyrme (zero-range) effective interaction
- Representation of single-particle wavefunctions on a 3D mesh
- Usually triaxial solutions with pairing
- Afterwards projection on good $\hat{J}$ and A
- Configuration mixing

Symmetries

$$\hat{P}, \hat{R}_z, \check{T}, \check{S}^T_y$$

$$\mathrm{DOF} = \begin{array}{l} \frac{1}{2} \times \mathrm{nx} \\ \frac{1}{2} \times \mathrm{ny} \\ \frac{1}{2} \times \mathrm{nz} \\ \frac{1}{2} \times \mathrm{nwt} \end{array}$$



Symmetries

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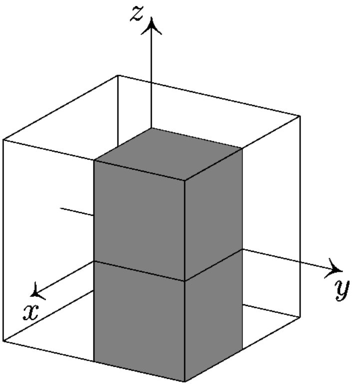
- ~~Parity~~

$$\mathrm{DOF} = \begin{array}{l} \frac{1}{2} \times \mathrm{nx} \\ \frac{1}{2} \times \mathrm{ny} \\ \quad\;\; \mathrm{nz} \\ \frac{1}{2} \times \mathrm{nwt} \end{array}$$



Symmetries

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- ~~Signature~~

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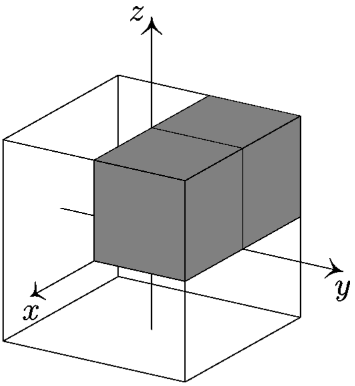
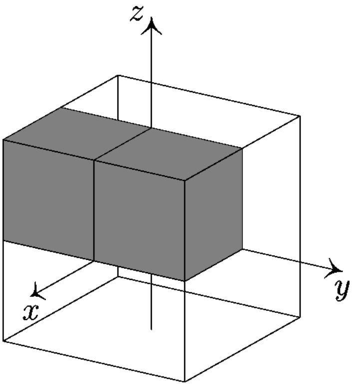


Symmetries

$$\hat{P}, \hat{R}_z, \check{T}, \check{S}_y^T$$

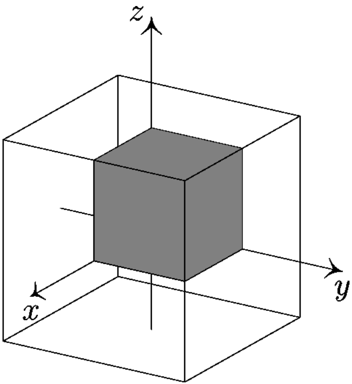
- ~~Time Simplex~~

$$\text{DOF} = \begin{array}{l} \frac{1}{2} \times \text{nx} \\ \quad\;\; \text{ny} \\ \frac{1}{2} \times \text{nz} \\ \frac{1}{2} \times \text{nwt} \end{array}$$



Symmetries

$$\hat{P}, \hat{R}_z, \check{T}, \check{S}_y^T$$



- ~~Time Reversal~~

$$\text{DOF} = \begin{array}{l} \frac{1}{2} \times \text{nx} \\ \frac{1}{2} \times \text{ny} \\ \frac{1}{2} \times \text{nz} \\ \quad\ \ \text{nwt} \end{array}$$

Pairing = Choice of quasiparticles

Hartree-Fock

$$\hat{\beta}^{\dagger}_{k} = \hat{\alpha}^{\dagger}_{k}$$

- No pairing

Pairing = Choice of quasiparticles

Hartree-Fock

$$\hat{\beta}_k^\dagger = \hat{\alpha}_k^\dagger$$

- No pairing

BCS

$$\hat{\beta}_k^\dagger = u_k \hat{\alpha}_k^\dagger + v_k \hat{\alpha}_{\bar{k}}$$

- Easy and (semi) free
- Not applicable without time-reversal

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HF-Bogoliubov

$$\hat{\beta}_k^\dagger = \sum_i u_i \hat{\alpha}_i^\dagger + v_i \hat{\alpha}_i$$

- Most general

MOCCa


```
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```

MOCCa = **Mo**dular **C**ranking **C**ode

MOCCa

- All symmetries ✓
- HF, BCS or HFB ✓
- Plenty Skyrme ✓
- Robust and easy ✓

```
        ;  ,
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```
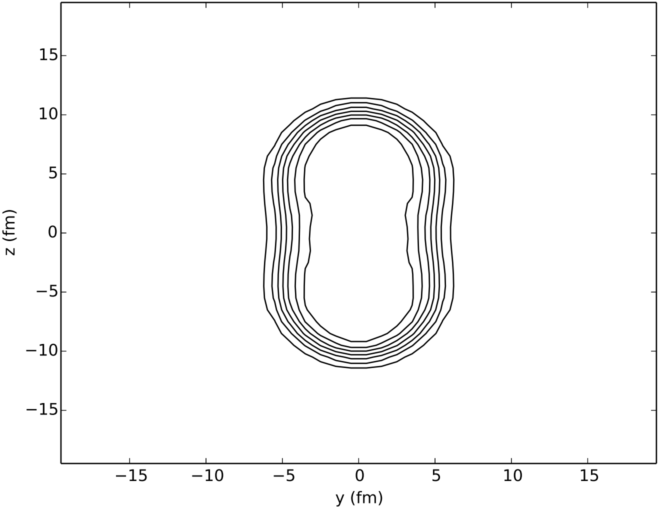
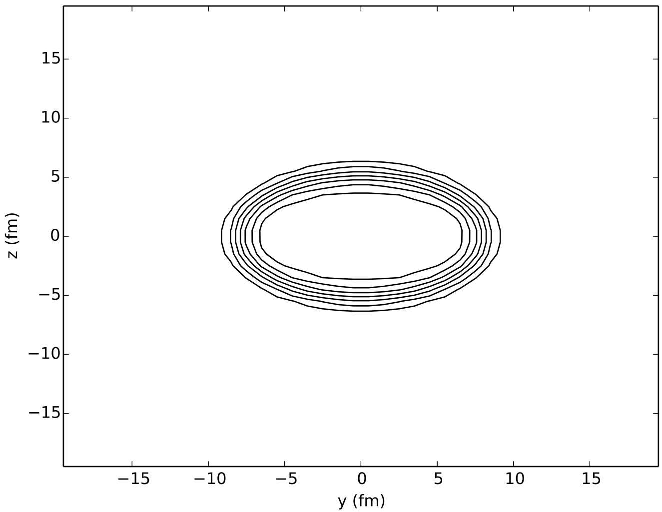

MOCCa = **Mo**dular **C**ranking **C**ode

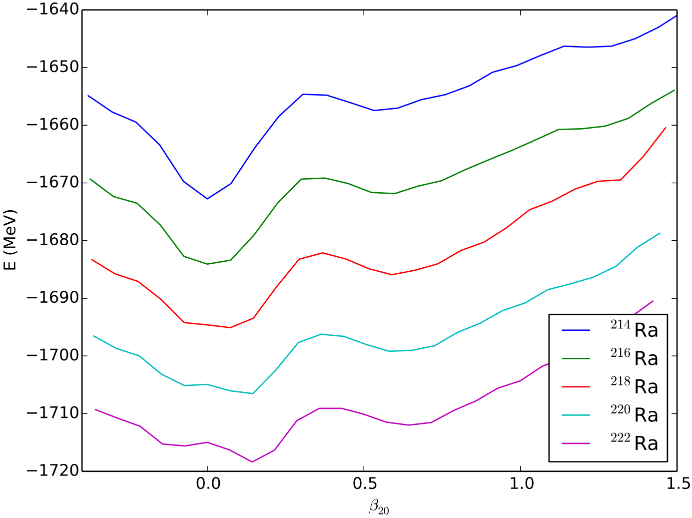
Rotational symmetry breaking



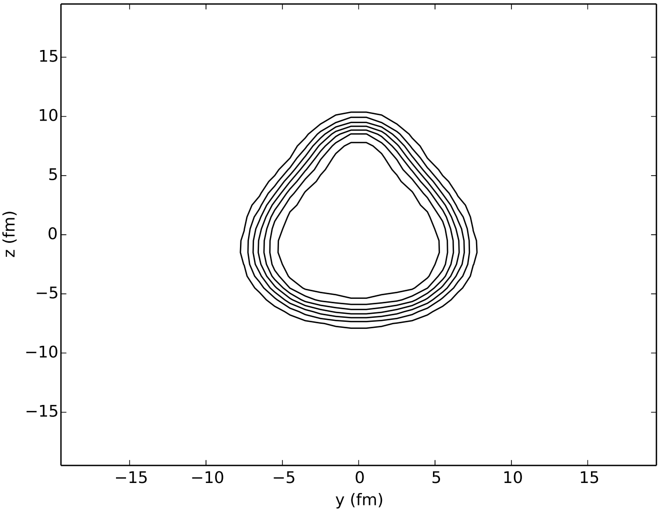
Rotational symmetry breaking



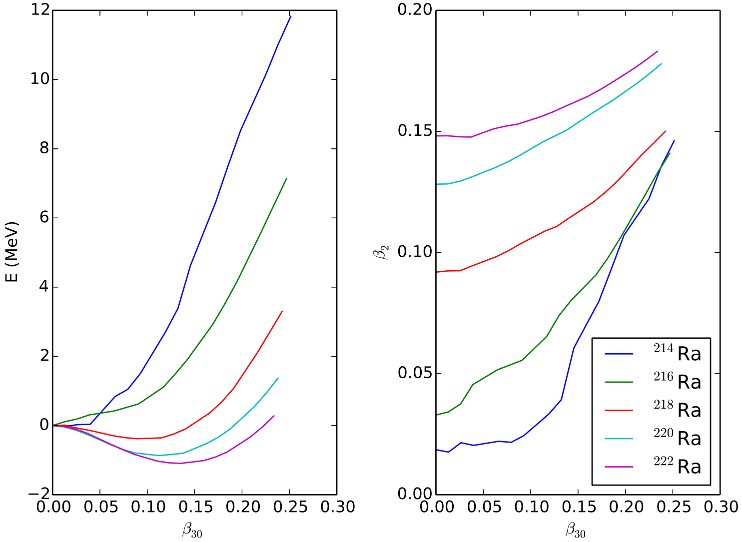
Radium Isotopes



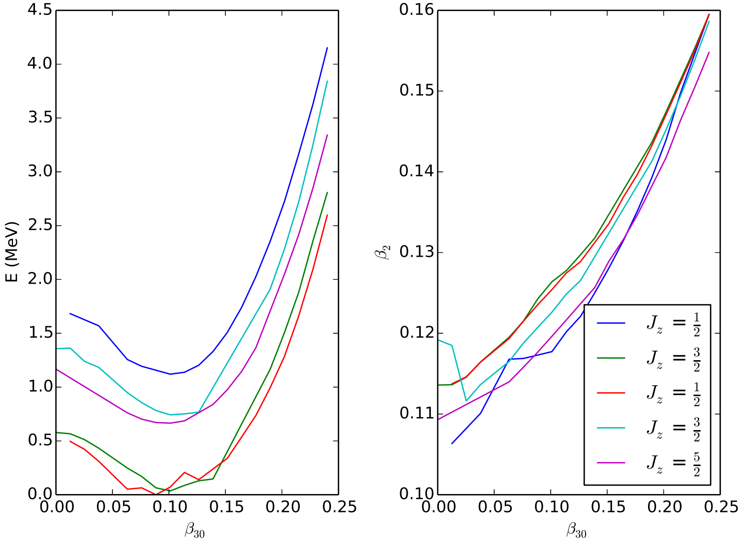
Parity



Radium Isotopes



^{219}Fr



E (MeV)
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.00
0.05
0.10
0.15
0.20
0.25
β_{30}
β_2
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.00
0.05
0.10
0.15
0.20
0.25
β_{30}
$J_z = \frac{1}{2}$
$J_z = \frac{3}{2}$
$J_z = \frac{1}{2}$
$J_z = \frac{3}{2}$
$J_z = \frac{5}{2}$

Conclusion

Last Time

- MOCCa: partial
- Applications are underway
- Future: HFB
- Far future: beyond-mean-field procedures

Now

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- MOCCa ✓

Conclusion

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- MOCCa ✓
- Full HFB ✓

Conclusion

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Now

- MOCCa ✓
- Applications are underway: Radium
- Full HFB ✓

Conclusion

Last Time

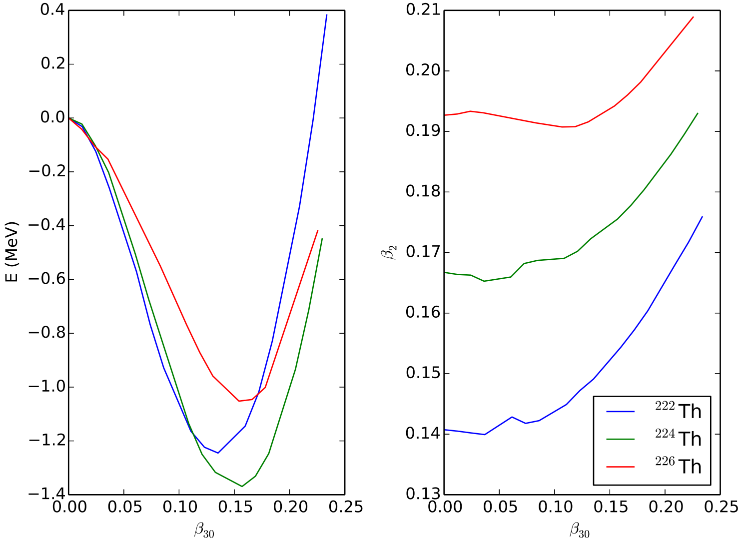
- MOCCa: partial
- Applications are underway
- Future: HFB
- Far future: beyond-mean-field procedures

Now

- MOCCa ✓
- Applications are underway: Radium
- Full HFB ✓
- Real close future: projection on parity

Thank you!

Thorium Isotopes



Octupole collectivity from a beyond-mean field point of view

V. Hellemans, M. Bender, P.-H. Heenen

Beyond mean-field approaches

Restrict form of the wavefunction to Slater determinant + break symmetries

↓

Symmetry restoration

↓

Configuration mixing

Mean-field approach : HF + BCS

Quasi-particle transformation :

$$\alpha_k^\dagger = u_k a_k^\dagger + v_k a_{\bar{k}}$$

$$|BCS\rangle \propto \Pi_i \alpha_i |0\rangle$$

↓

$$\mathcal{E} = \mathcal{E}_{\text{kin}} + \mathcal{E}_{\text{Sk}} + \mathcal{E}_{\text{pairing}} + \mathcal{E}_{\text{Coulomb}}$$

$\delta\mathcal{E} = 0$ → ground state

describe a ground state of pairwise interacting states as a gas of non-interacting quasi-particles

Pairing of p-p correlations included !

no longer good particle number !

Mean-field approach : HF + BCS

Quasi-particle transformation :

$$\alpha_k^\dagger = u_k a_k^\dagger + v_k a_{\bar{k}}$$

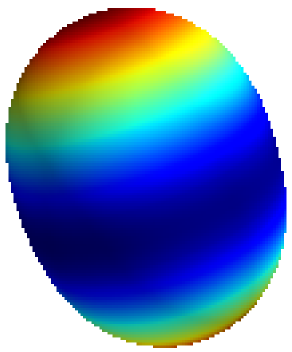
$$|BCS\rangle \propto \Pi_i \alpha_i |0\rangle$$

$$\mathcal{E} = \mathcal{E}_{\text{ kin}} + \mathcal{E}_{\text{Sk}} + \mathcal{E}_{\text{pairing}} + \mathcal{E}_{\text{Coulomb}}$$

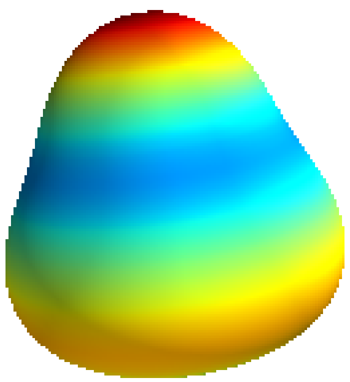
$$\delta(\mathcal{E} - \lambda_N \langle \hat{N} \rangle - \lambda_N \langle \hat{Z} \rangle) = 0$$

describe a ground state of pairwise interacting states as a gas of non-interacting quasi-particles

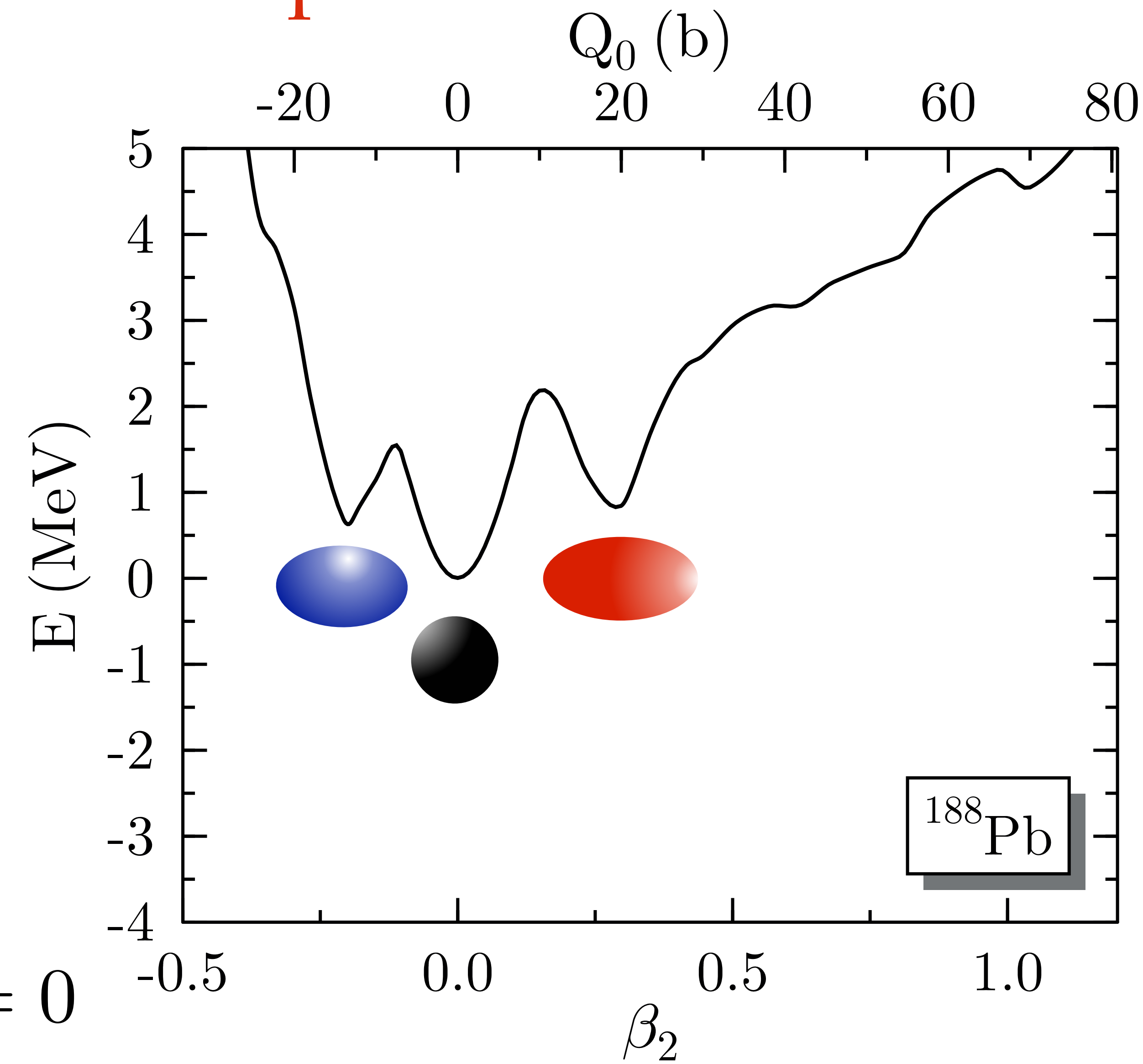
How to include deformation in this picture ?



(2,0)
rotational symmetry broken



(3,0)
parity broken



$$\delta(\mathcal{E} - \lambda_N\langle\hat{N}\rangle - \lambda_Z\langle\hat{Z}\rangle - \lambda_q\langle\hat{Q}_{lm}\rangle) = 0$$

Breaking of rot. symmetry => the np-nh SM correlations

Symmetry breaking allows us to take extra (static) correlations into account w/o losing the simple independent (quasi) particle picture

M. Bender *et al.*, PRC 69, 064303 (2004)

Beyond mean-field : symmetry restoration

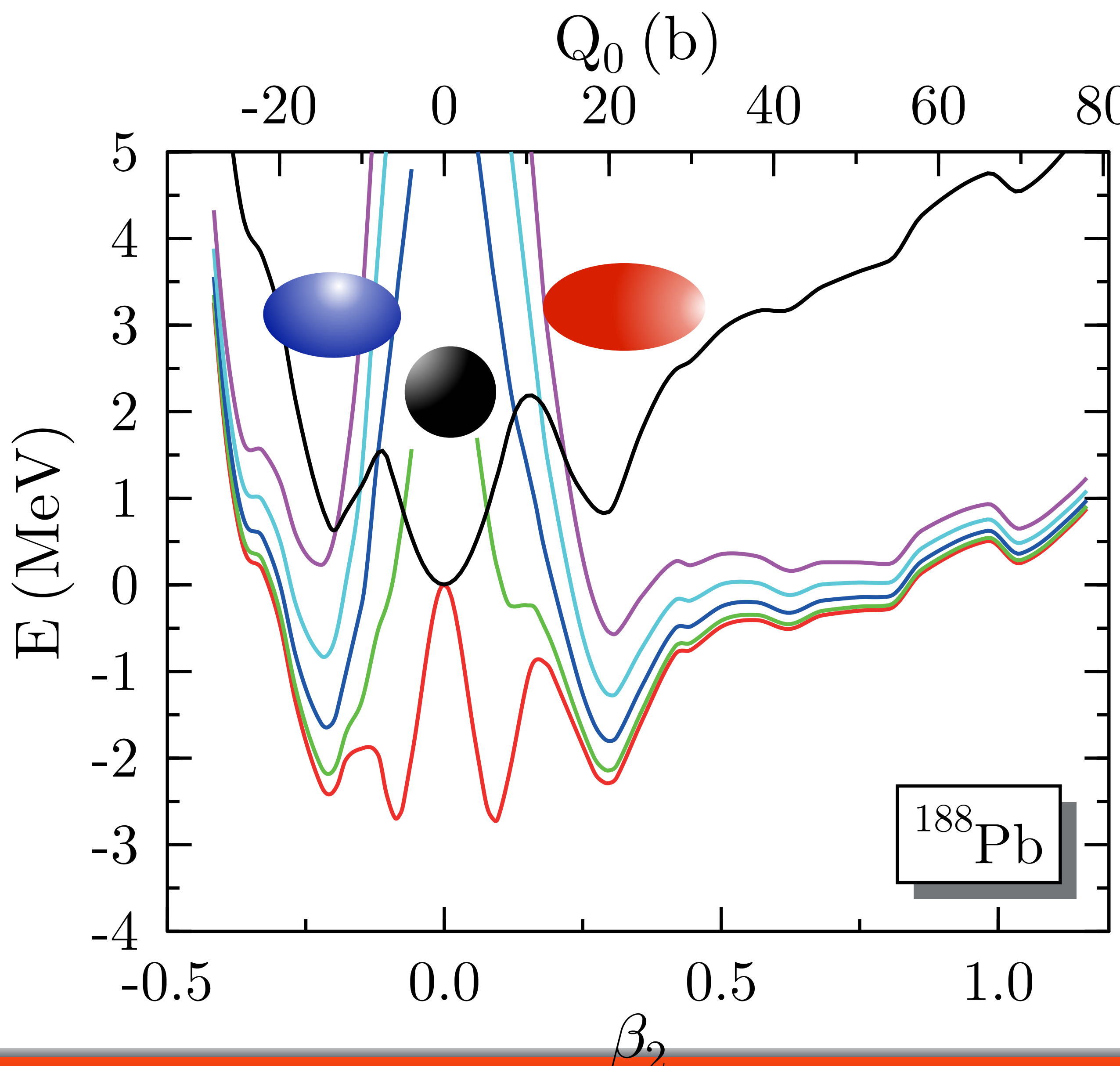
$$|JMq\rangle = \frac{1}{\mathcal{N}_{JMq}} \hat{P}^{J}_{M0} \hat{P}_{Z} \hat{P}_{N} \hat{P}^{\pi} |q\rangle$$

axial symmetry

Ang. momentum projection

$$\hat{P}^{J}_{M0} = \frac{2J+1}{16\pi^2} \int d\Omega D^{J*}_{M0} R(\Omega)$$

- mixes states with different orientations
- leads to enriched wavefunction that contains more correlations than | q>



M. Bender *et al.*, PRC 69, 064303 (2004)

Beyond mean-field : configuration mixing

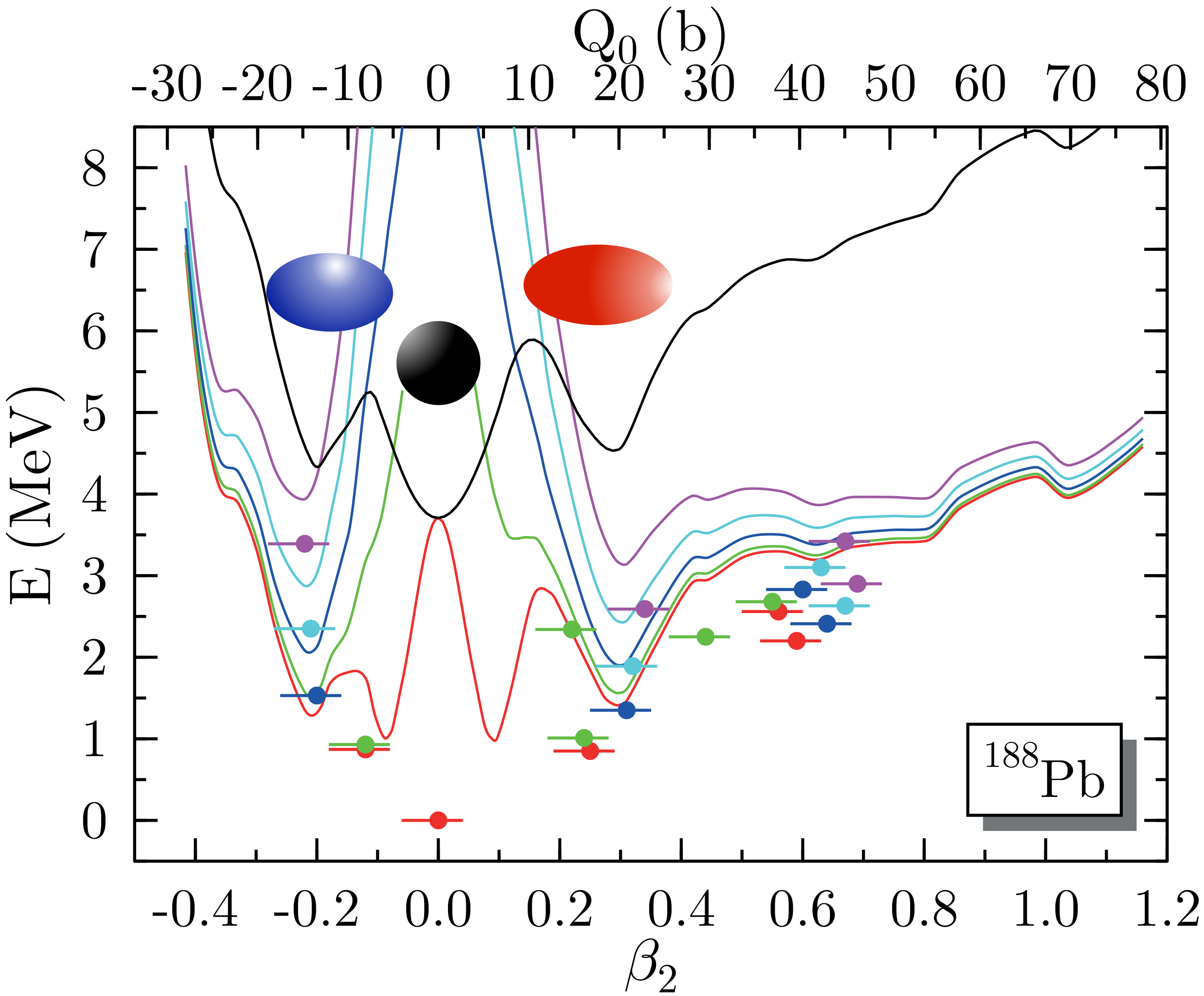
$$|JMk\rangle = \sum_q f_{J,k}(q)|JMq\rangle$$

$$\delta\langle JMk|H|JMk\rangle = 0$$

HW equations

- Superposition of many symmetry projected mean-field states

Dynamical correlations: collective correlations around a given mean-field state



M. Bender *et al.*, PRC 69, 064303 (2004)

Beyond mean-field : configuration mixing

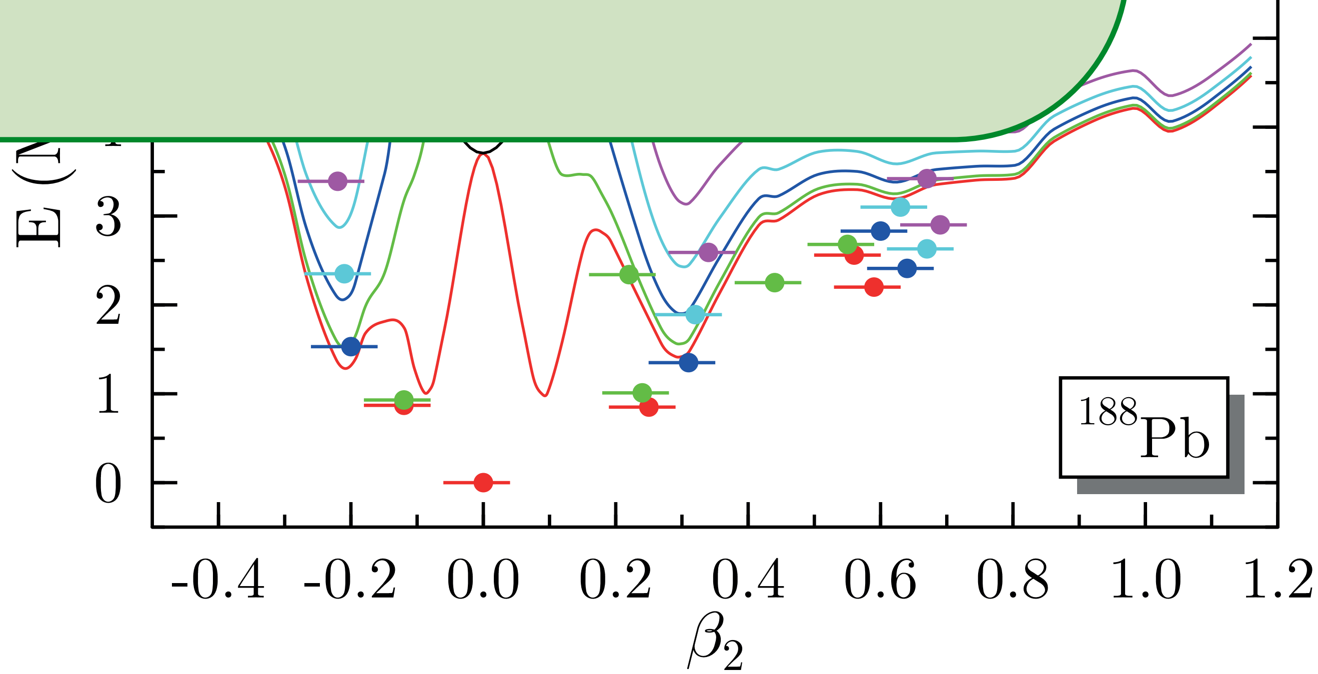
$$|JMk\rangle = \sum_q f_{J,k}(q)|JMq\rangle \quad \Rightarrow \quad \delta\langle JMk|H|JMk\rangle = 0$$

HW equations

Thus far limited to quadrupole deformed nuclei

Present: octupole collectivity

collective correlations around a given mean-field state

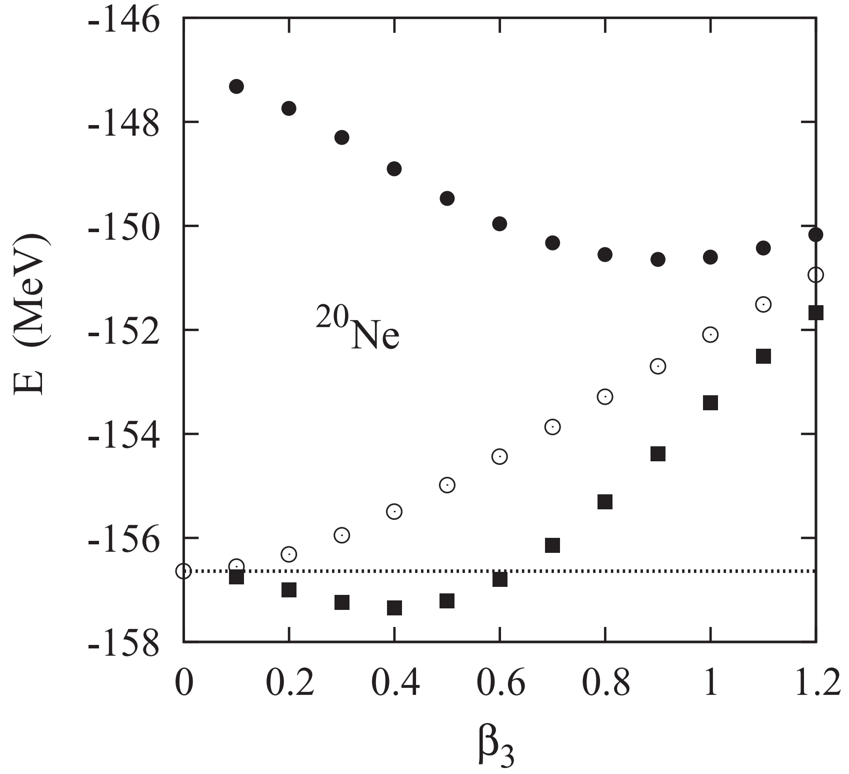


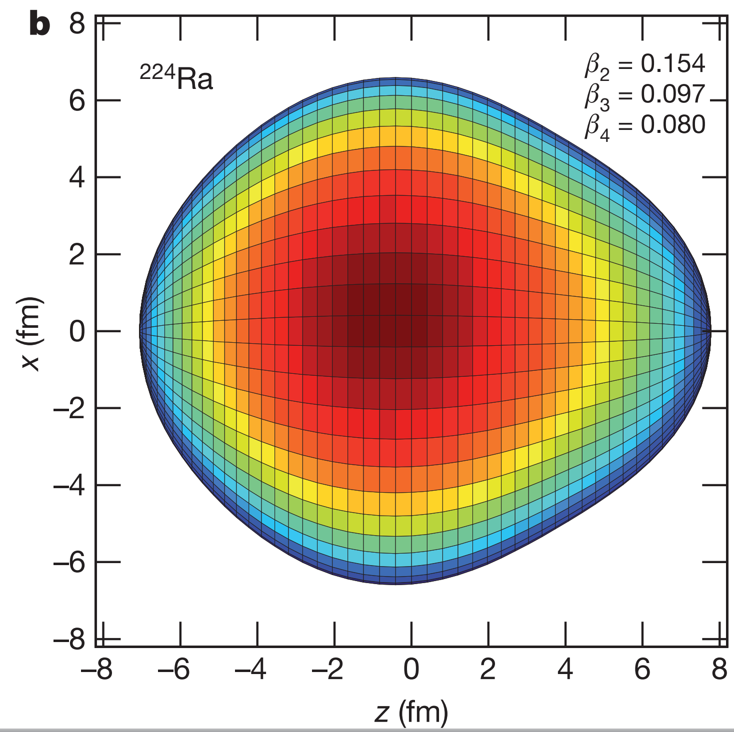
M. Bender *et al.*, PRC 69, 064303 (2004)

Octupole collectivity

Some phenomena require the inclusion of octupole deformation in (beyond) mean-field approaches

- Asymmetric fission
- E1 transitions (! nucleosynthesis)
- Nuclei with static octupole deformation (e.g. Ra) or octupole deformation after PP (eg. 20Ne)
- Such nuclei are important in search for permanent atomic E1 moment

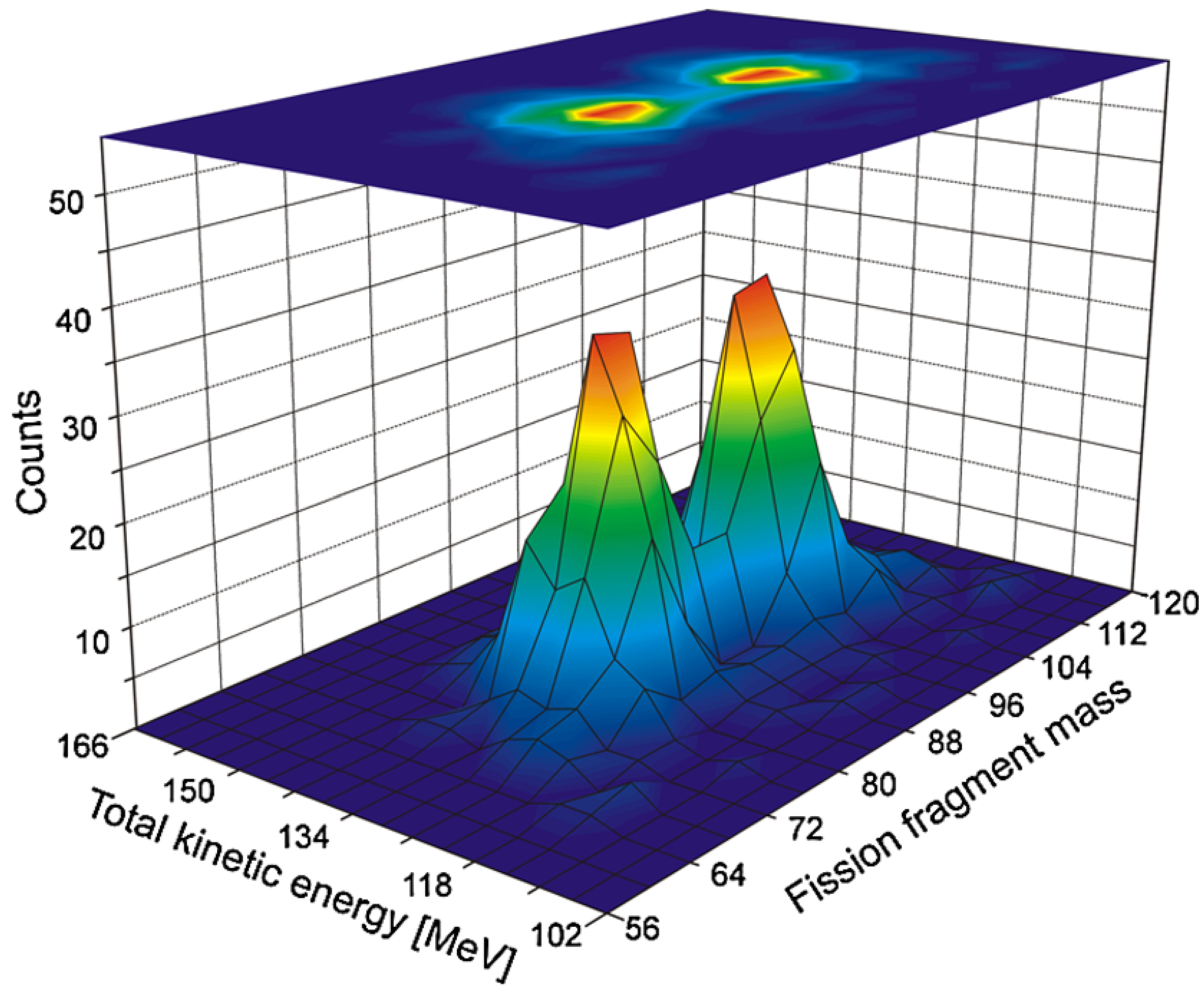




L. Robledo *et al.*, PRC 84, 054302, 2011

L. Gaffney *et al.*, Nature 497,2013

^{180}Hg: asymmetric fission



A. Andreyev *et al.*, PRL 105, 252502, 2010

$$\beta_l = \frac{4\pi}{3AR^l} \int d^3r \; r^l Y_{l0} \rho$$

Static mean-field approach to ^{180}Hg

Theoretical fission barrier too high, even after projection

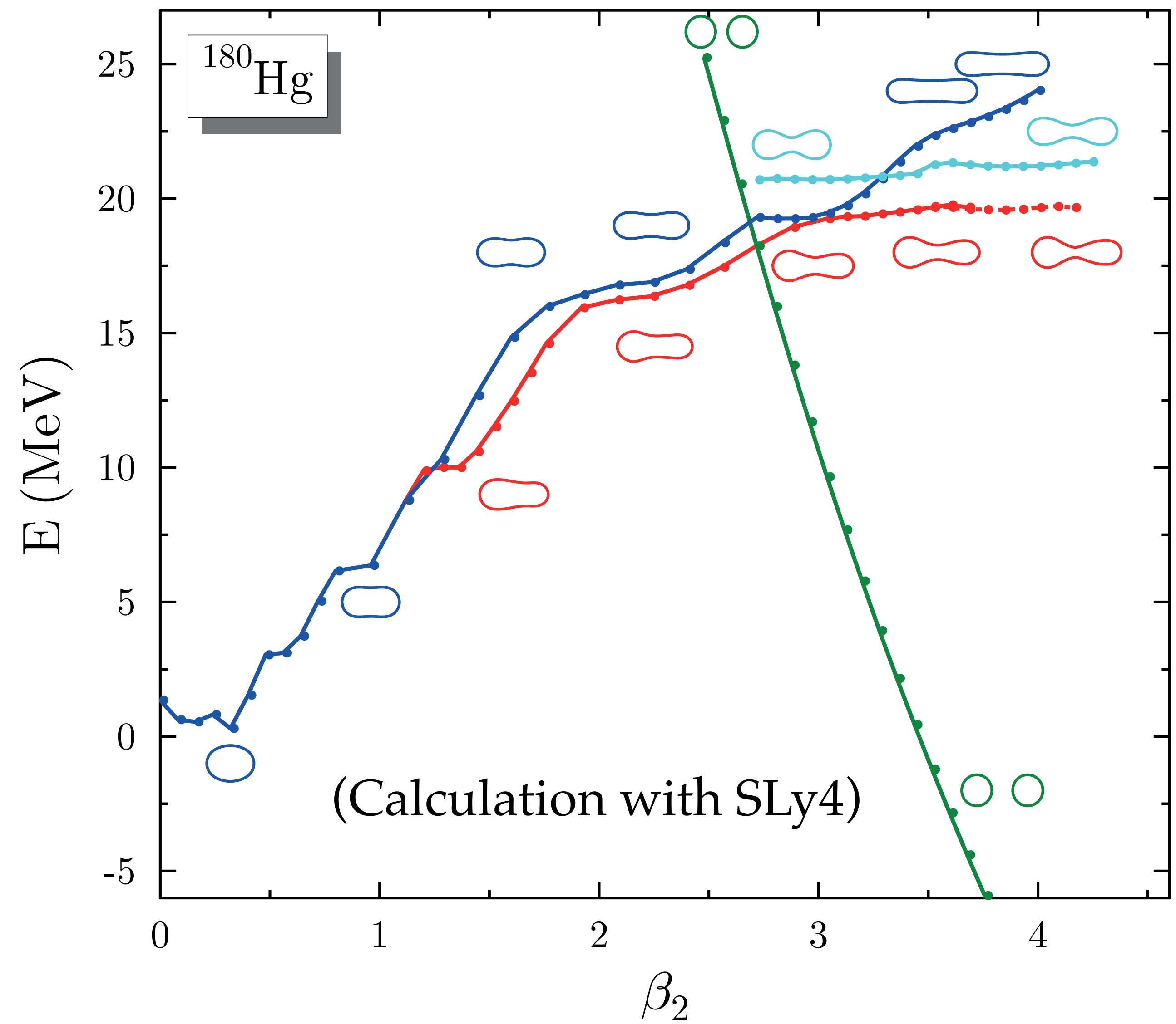
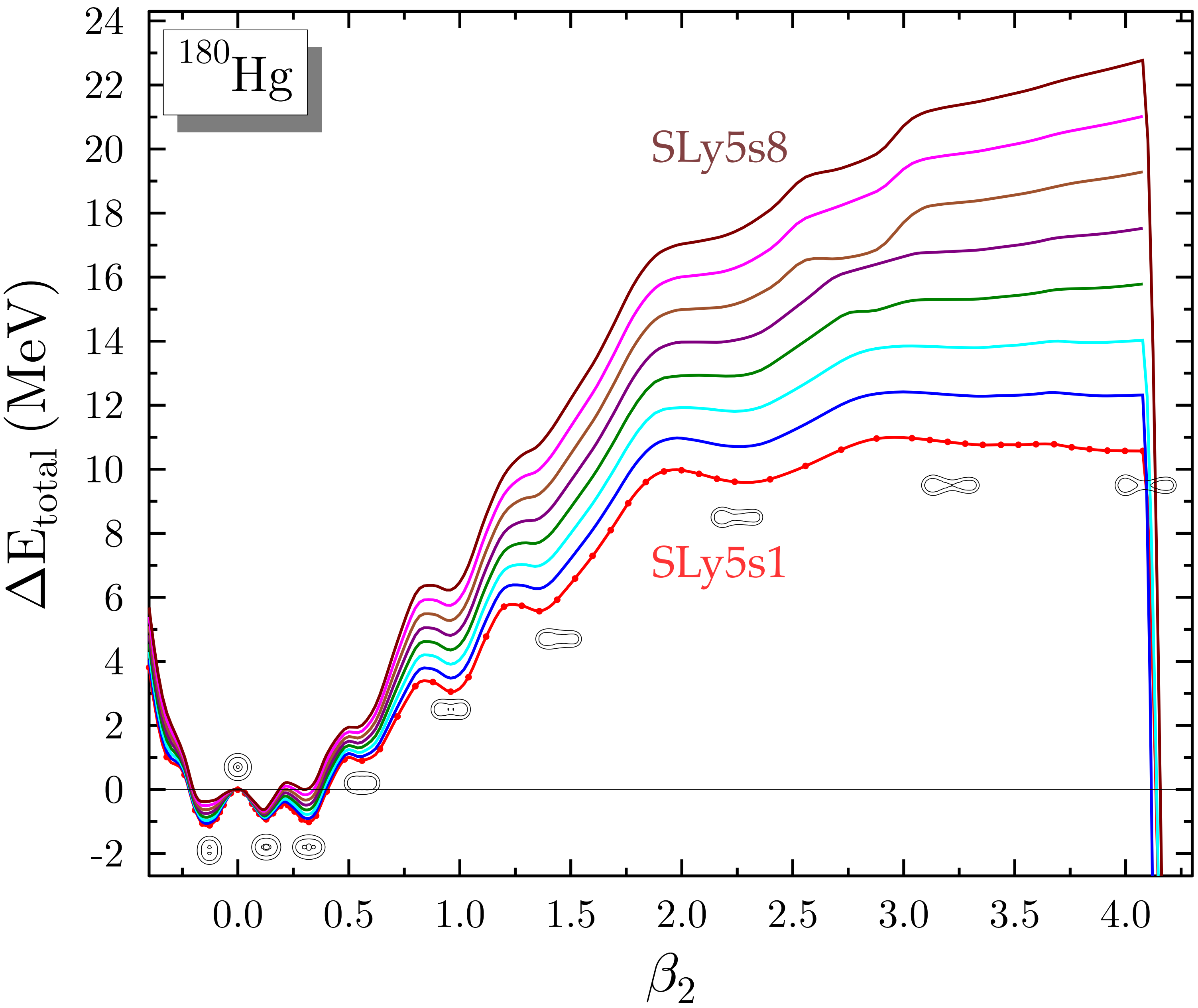
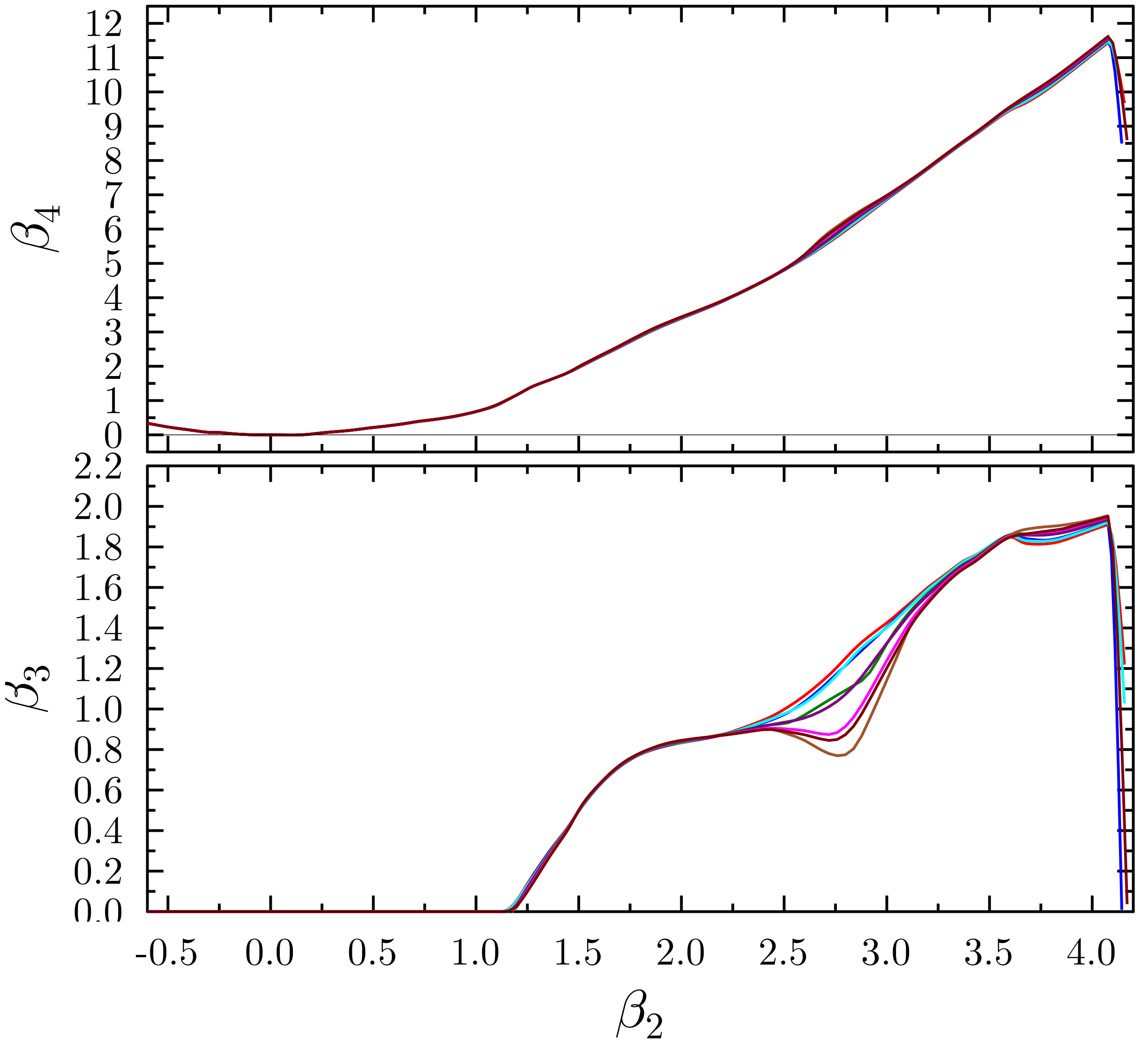


Figure courtesy M. Bender

New SLysX Skyrme interactions



- Set of Skyrme parametrizations for which the surface parameter is varied in a controlled way (R. Jodon, K. Bennaceur, J. Meyer)

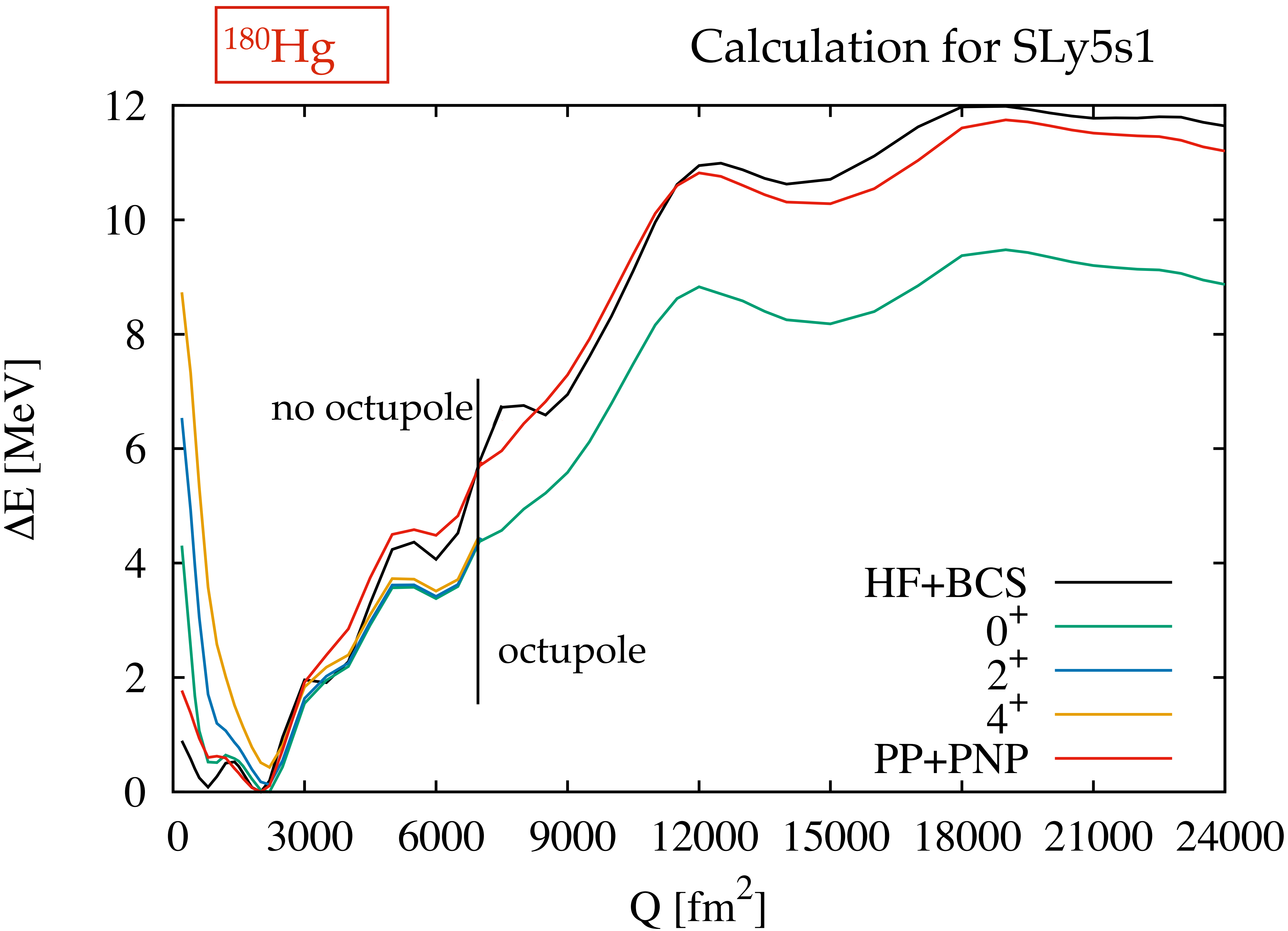


^{180}Hg

- Lower a_s - improved results

Figure courtesy M. Bender

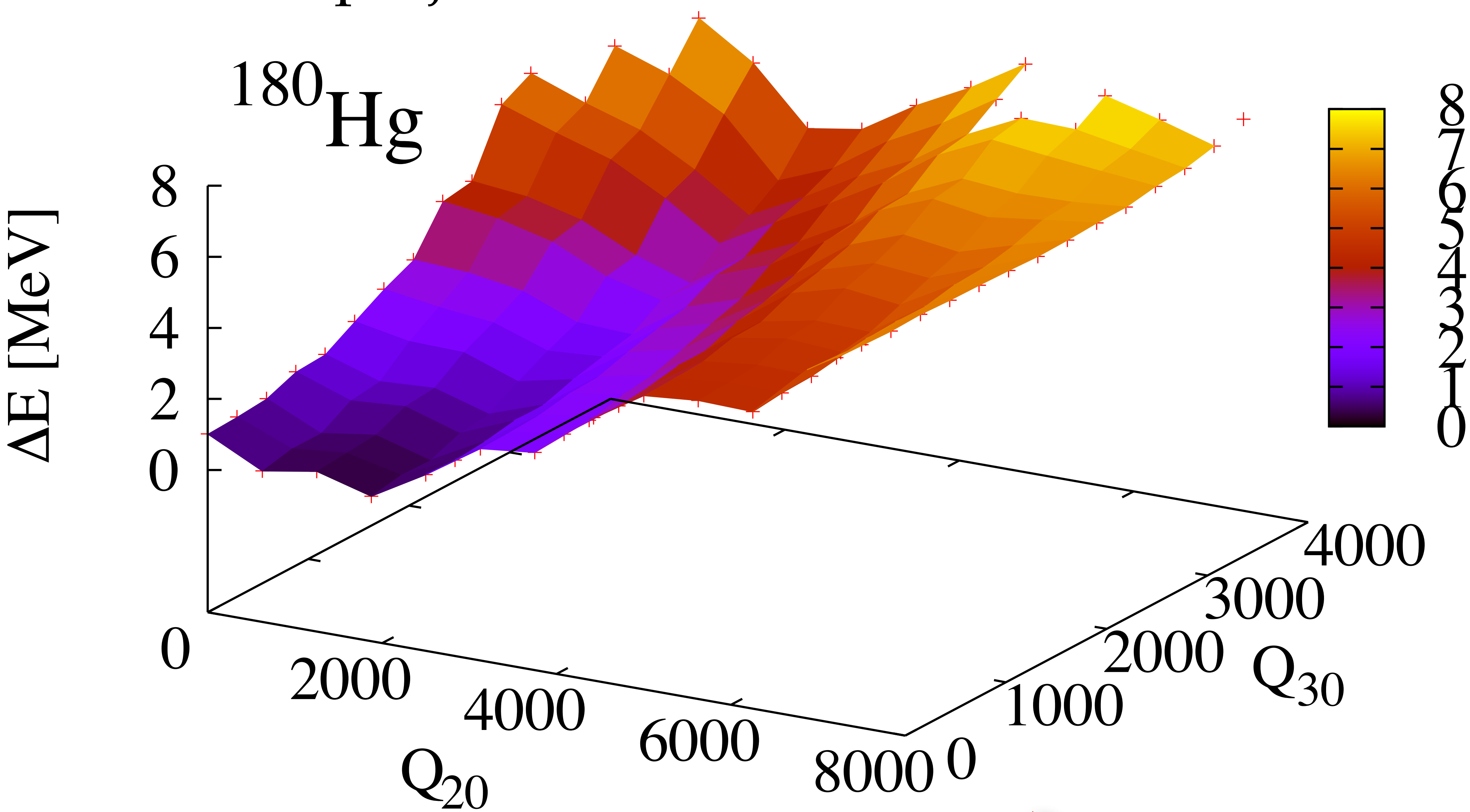
ULB ⋮ ^{180}Hg : projection on AMP+PP+PNP



^{180}Hg : projection on AMP+PP+PNP

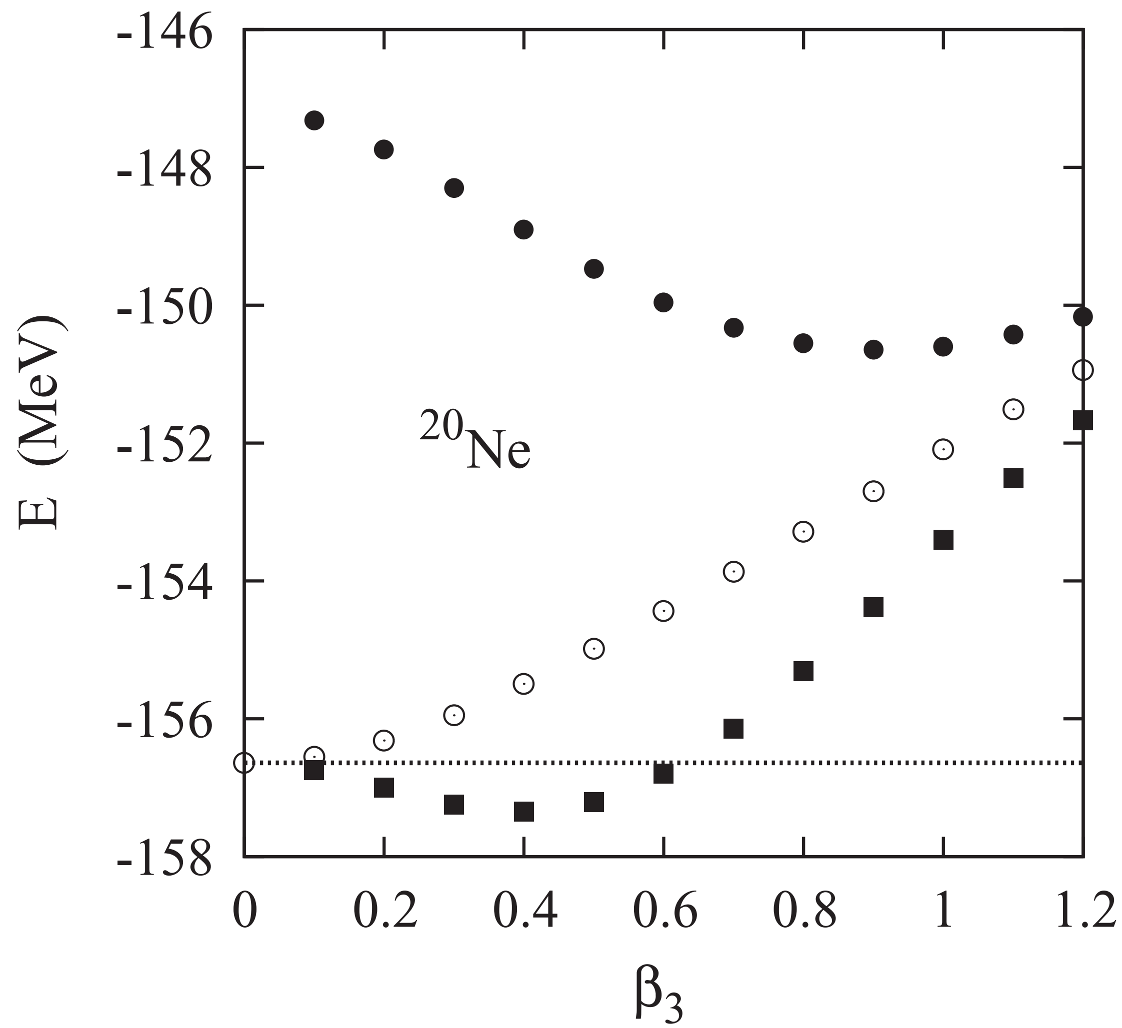
^{180}Hg

=> thus far : only "minimal path" at mean-field level projected. The full q2-q3 surface needs to be constructed to find the "minimal path" after projection

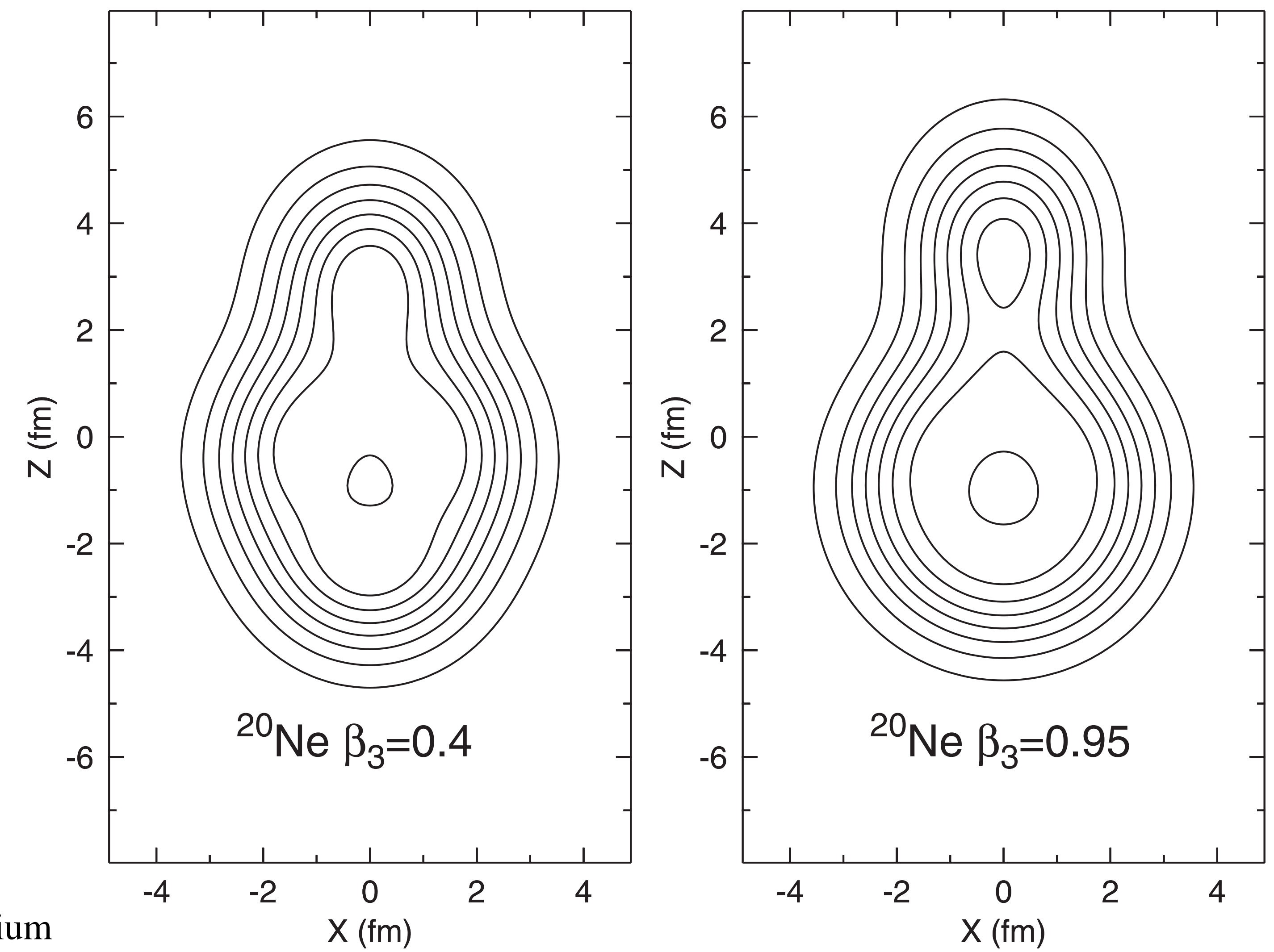


Numerically expensive

^{20}Ne - a full GCM perspective

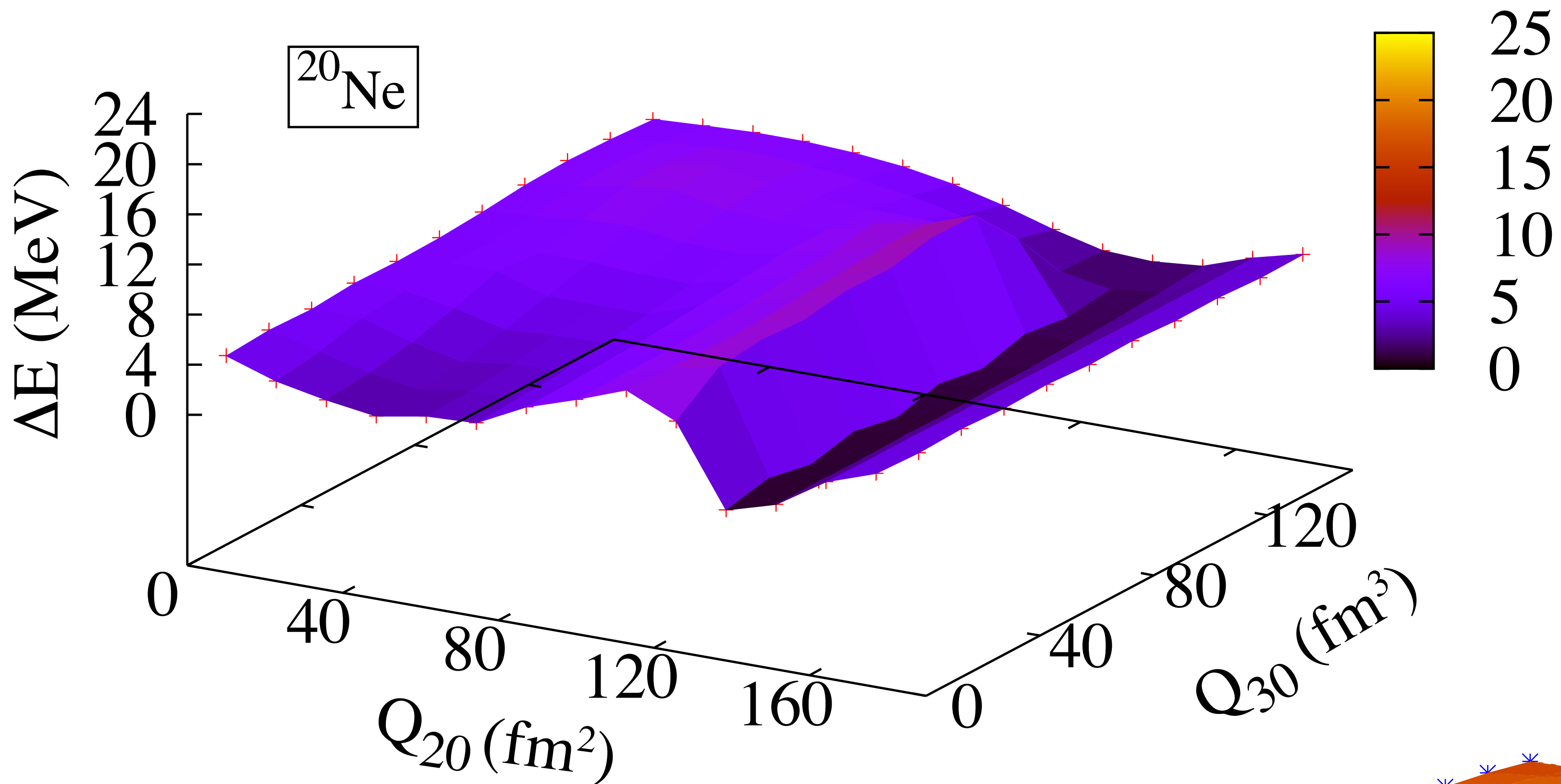


Ref. [1]. Due to the incipient alpha clustering, the equilibrium octupole deformation of the projected configurations can be very large. The HFB and projected energies are shown in Fig. 6. Note that the HFB energy deviates from a quadratic dependence on the deformation, and looks almost linear at large β_3. Figure 7 shows the density distribution at the two projected minima. One sees a compact localized density, suggestive of an alpha particle, outside a nearly spherical core. Since the α emission threshold is rather low in this



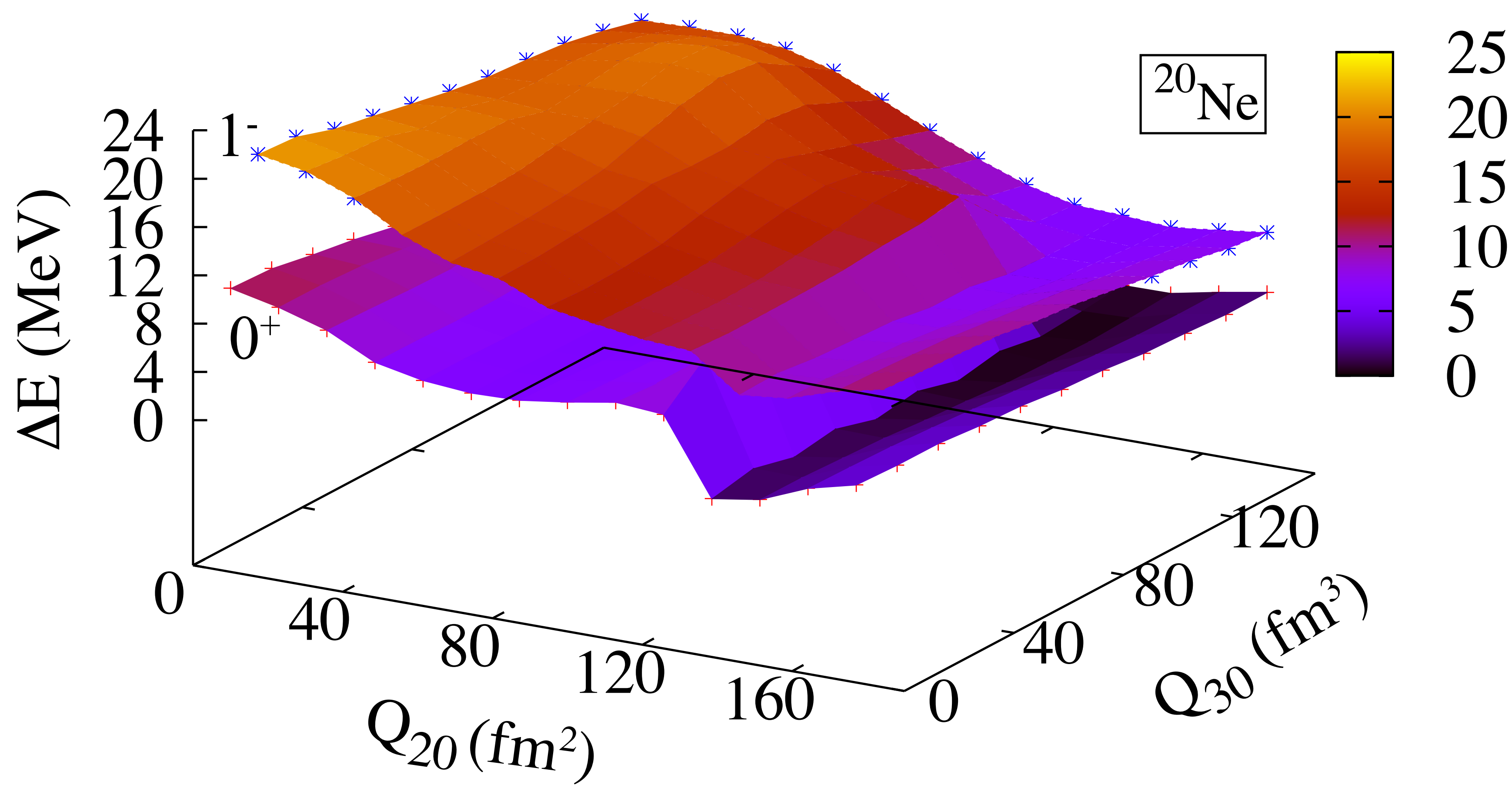
L. Robledo *et al.*, PRC 84, 054302, 2011

^{20}Ne : full GCM

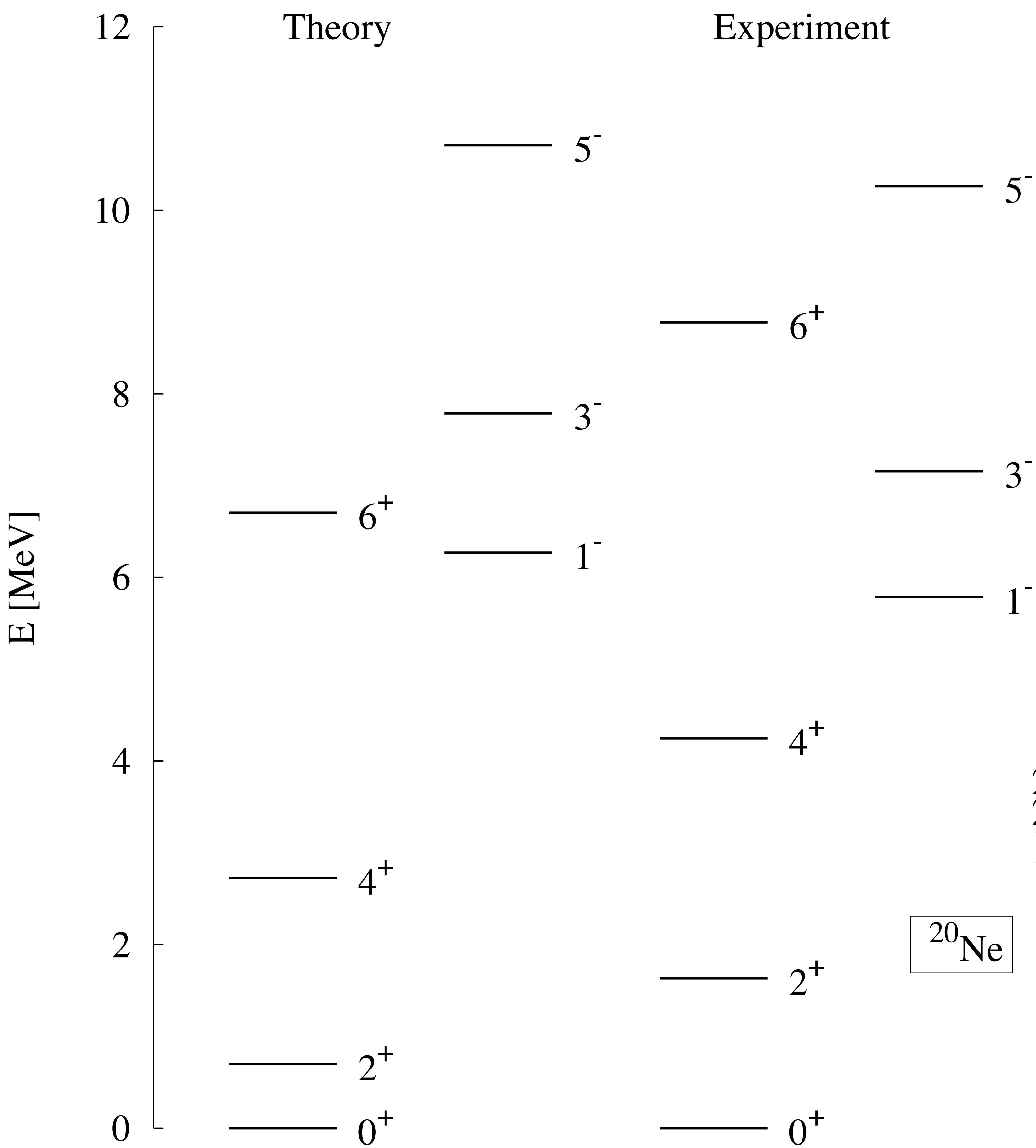


- no pairing, only HF
- SLy5 Skyrme interaction

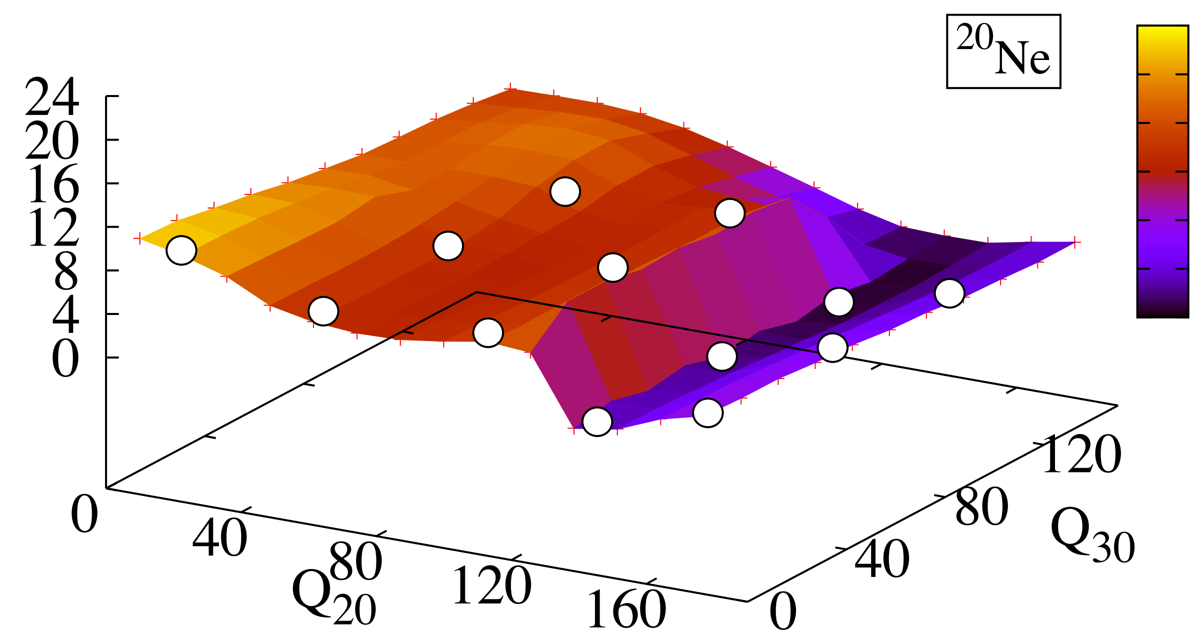
- Octupole deformed minimum after PP+ +AMP projection



^{20}Ne : full GCM



- Configuration mixing after parity and J-projection
- Q_{20} and Q_{30} degrees of freedom
- $Q_s(2_1)$=-18.7 e fm^2 (exp 18.0 ± 2.0 e fm^2)



ULB Conclusions and outlook

- The new SLy5s(1-8) parametrization are promising for the description of fission barriers
- A more systematic study of PP+PNP+AMP projected barriers should be performed to decide which SLy5s(1-8) is the best.
- First GCM with AMP+PP projected octupole deformed states for ^{20}Ne

➡ To do ?

- Still implement EM (dipole,quadrupole,octupole, ..) transitions in the Hill-Wheeler code for configuration mixing
- **Tackle the physics !!**

Thanks to my collaborators

- P.-H. Heenen, W. Ryssens (ULB, Brussels)
- M. Bender (CENBG, Bordeaux)
- R. Jodon, J. Meyer (Lyon)
- K. Bennaceur (Jyväskylä)

Thank you for your attention !